Effect of electric fields on the reaction rates in shock initiating and detonating solid explosives

Craig M. Tarver

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EFFECT OF ELECTRIC FIELDS ON THE REACTION RATES IN SHOCK INITIATING AND DETONATING SOLID EXPLOSIVES

Craig M. Tarver

Lawrence Livermore National Laboratory, Livermore, CA 94550

Abstract. The presence of a strong electric field has been demonstrated to effect the shock initiation and detonation wave propagation of solid high explosives. Several mechanisms have been proposed to explain the observed increased shock sensitivity, increased detonation velocity, and decreased failure diameter of certain explosives. The most likely chemical mechanism is postulated to be the excitation of some of the explosive molecules and/or intermediate reaction products to higher energy electronic states, which rapidly transition nonradiatively to the ground electronic state with excited vibrational states. This vibrational excitation increases the reaction rates of the explosive decomposition chain reactions. The resulting shorter duration reaction zone causes faster shock to detonation transition, decreased failure thickness, and increased detonation velocity for a specific charge diameter.

Keywords: Detonation, shock initiation, electric field effects

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INTRODUCTION

Tasker et al. [1] reviewed the experimental evidence for effects of electric and magnetic fields on shock initiation and detonation in solid explosives. They concluded that magnetic fields as strong as 1 Tesla have no effect on the shock initiation and detonation of solid explosives. Since embedded electromagnetic particle velocity gauges are used in 0.1 Tesla fields, these magnetic fields do not affect the evolving reactive flows.

Strong electric fields have been shown to affect shock sensitivity and detonation [1]. Initially, it was believed that electrically conducting reacting explosives in shock or detonation waves could absorb large quantities of electrical energy, which would then act like chemical energy and greatly increase the power of detonating explosives. Estimates made using simple energy arguments [2] and joule heating assumptions in the chemical equilibrium code TIGER [3] resulted in very high detonation velocities

and Chapman-Jouguet (C-J) pressures. These extreme states have not been observed, but three cases of increased shock initiation and/or detonation reaction rates have been reported. R. Lee et al. [4] demonstrated that a 5 kV voltage electric field applied to 88% HMX/12% HTPB explosive charges increased their shock sensitivity by measuring back surface blow off velocities as functions of time and input shock pressure. J. Lee et al. [5] observed increased detonation velocities in 2 mm thick primasheet charges subjected to 5 kV voltages. Winter et al. [6] showed that the failure diameters of wedges of EDC35 (95% TATB and 5% Kel-F binder) were reduced by applying electrical fields exceeding certain minimum strengths.

Tasker et al. [1] also offered several possible explanations of the electric field effect. These included: bulk heating of the reaction products by Joule heating; reduction of the energy barrier that facilitates dislocation motion; perturbations to the chemical reaction activation energy; and acceleration of plasma projected from the reaction zone. Other explanations have also

been proposed, as summarized by Kuklja [7]. This paper provides a proven chemical kinetic explanation of the electric field effect.

ELECTRICAL CONDUCTION IN THE REACTING EXPLOSIVE MIXTURE

For the electrical energy to affect a shocked reacting explosive, it must first be conducted the reacting chemical mixture. Unreacted organic explosives are extremely poor electrical conductors [8]. Time resolved measurements of detonating solid explosives from Hayes' classic experiments [8] to recent studies [9-11] have shown that the amount of electrical conduction in a detonation wave is directly proportional to the amount of solid carbon produced during the chemical decomposition. Gorshkov et al. [11] measured peak conductivity in a TATB detonation wave about one microsecond behind the shock front followed by a decrease attributed to the growth of solid carbon nanoparticles. Gaseous reaction products do not conduct electricity well, and thus detonation waves in nearly oxygen balanced explosives such as PETN show extremely small values of electrical conductivity [8].

CHEMICAL REACTION RATES

Once the solid carbon products have conducted significant electrical energy, how can this affect the chemical reaction rate of the reacting mixture? Joule heating has been ruled out as not being sufficiently strong in the microseconds or less available to affect energy release [1]. An efficient chemical process is the excitation of various molecular species from the ground electronic state to the first (or higher) excited electronic state. This excitation has been shown experimentally [12] and theoretically [13] to be followed within picoseconds by a nonradiative transition back to the ground electronic state accompanied by excitation of that state's vibrational levels. The highly vibrational excited molecules undergo more frequent reactive collisions than those in lower vibrational states [14], thus increasing the

chemical energy release rate and reducing the overall reaction zone length of the detonation wave [14] or lower pressure chemical processes [15]. A simplified reaction sequence is:

Electrons + M
$$\longrightarrow$$
 M*^{Elec} (1)

$$M^{*Elec} \longrightarrow M^{*Vib}$$
 (2)

$$A + M^{*Vib}$$
 ---> Products (3)

where M and A are explosive or intermediate product molecules, *Elec denotes electronic excitation, and *Vib denotes high vibrational excitation of the ground electronic state.

Since the detonation reaction length controls the detonation velocity versus inverse charge radius relationship [16], an electronically excited explosive charge of a certain diameter can exhibit a higher detonation velocity and smaller failure diameter. The total amount of additional energy from electronic excitation is small with respect to the exothermic chemical energy, but it is effective in increasing the overall rate of the chemical energy release.

In a detonation wave of rich carbon explosive such as TATB, the carbon coagulation process accounts for much of the reaction time [17]. TATB's stoichiometric balance is:

$$C_6H_6N_6O_6--->3$$
 N_2 +3 H_2O +3/2 CO_2 +9/2 C (4)

The reaction zone length of detonating TATB is known to be 3 mm or 400 ns [17,18]. The rapid formation of stable gaseous products such H_2O , CO_2 , N_2 , CO, and carbon normally requires 80 ns. This process can be accelerated by electrical excitation. The remaining 320 ns of diffusion controlled carbon nanoparticle coagulation may or may not be affected by the presence of the electric field, but the total reaction time may be shortened enough to cause observable effects.

SLOW FAILURE IN EDC35 WEDGES

Winter et al. [6] measured detonation failure thicknesses of EDC35 wedges of: 3.2 mm when no electrical energy was applied; 3.1 mm when

25 kV, 1.25 kJ was applied, and 2.7 mm when 25 kV, 5 kJ was applied. Using the LANL prism test, Ramsay [19] showed that the failure thicknesses of PBX 9502 (95% TATB/5% Kel-F) wedges are reduced significantly by thin confinement layers, which decrease reaction zone lengths. Asay McAfee [20] produced thicknesses of 2 mm by preheating unconfined PBX 9502 wedges to 173°C or 250°C. A higher initial temperature shortens the overall reaction time. Garcia and Tarver [21] applied the 3D PBX 9502 Ignition and Growth reactive flow model to unconfined, confined, and preheated prism tests. obtain a calculated failure thickness of 2.7 mm, the coefficient G₁, which controls the rate of formation of the gaseous species, had to be increased from 4613 to 7200. This change reduced the time required for that reaction from 80 us to approximately 50 us. The ability of excess vibrational energy to accelerate exothermic chain reaction mechanisms in the electric field experiments can account this factor of 1.6 increase in the main chemical reaction rate of EDC35.

DETONATION IN PRIMASHEET

J. Lee et al. [5] measured average detonation velocity increases of 2.7-3.2% and local jumps of 8.2-10.4% in 2 mm thick primasheet, which is very similar to detasheet. Since the main explosive in this sheet explosive is PETN, which has a reaction zone of only a few ns and a failure diameter well below 1 mm, and whose products conduct very little electricity [8], how could electric fields affect the detonation velocity of primasheet? Primasheet contains only 63% by weight PETN, 8% nitrocellulose $(C_6H_{7.74}N_{2.26}O_{9.52})_n$, and 29% acetyl tributyl citrate ATBC $(C_{20}H_{34}O_{8})_m$. Thus primasheet's stoichiometric balance is approximately:

$$C_{118}H_{194}N_{34}O_{133}--->$$

$$17 N_2 + 97 H_2 O + 18 CO_2 + 100 C$$
 (5)

This decomposition produces a high percentage of solid carbon. Thus primasheet reaction products can conduct electricity, and primasheet has a longer reaction zone and larger failure diameter than pure PETN. As in detonating TATB, electrical excitation in detonating primasheet can produce a shorter reaction time, a smaller failure diameter, and an increase in detonation velocity from 7 to 7.2 km/s, which is close to its C-J velocity, in 2 mm thick charges.

SHOCK INITIATION OF HMX/HTPB

HMX has a better oxygen balance than TATB and primasheet and thus produces much less solid carbon during its chemical decomposition [10]. 12% HTPB binder increases the amount of carbon and hydrogen present when mixed with 88% HMX. This increases the amount of solid carbon formed during shock initiation and detonation, because oxygen reacts with hydrogen to form water rather than form CO₂ with carbon. Thus there is a significant amount of solid carbon present in the shocked, reacting region of R. Lee et al.'s [4] experiment. Although the pressures and temperatures are lower than those of a detonation wave, conduction of electrical energy can occur over a larger volume and a longer time (several µs). The absorption of electrical energy can increase the overall reaction rate, thus resulting in the measured faster growth of hot spot reactions and a more rapid transition to detonation.

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